Charge Transfer Between Neutral Atoms and Highly Ionized Species: Implications for ISO Observations

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ABSTRACT

We estimate rate coefficients for charge transfer between neutral hydrogen and helium and moderate to highly ionized heavy elements. Although charge transfer does not have much influence on hot collisionally ionized plasmas, its effects on photoionized plasmas can be profound. We present several photoionization models which illustrate the significant effect of charge transfer on the far infrared lines detected by ISO.

Subject headings: atomic data — atomic processes — infrared: spectra

1. Introduction

The ionization balance of the elements in an ionized gas is determined by photoionization and particle impact ionization and radiative, dielectronic and three-body recombination. If the gas contains a neutral component, charge transfer recombination may occur. In a high temperature plasma in which ionization is produced mainly by thermal collisions of electrons, charge transfer is rarely of significance for highly ionized species because the abundance of neutral systems is very small. However, in plasmas in which ionization is produced by high frequency photons, a significant abundance of neutral hydrogen and helium atoms may co-exist with multiply-ionized heavy elements.

2. Charge transfer

Because many states are energetically accessible for ions of high nuclear charge colliding with neutral atoms, it can be argued that electron capture by the ion is inevitable, occurring on every collision. The electron transfer takes place at distances where the interaction is determined by the polarization of the atom by the electric field generated by the approach of the ion.

If we assume that every collision that surmounts the centrifugal barrier leads to a reaction, we obtain the Langevin formula

$$\sigma = \pi\zeta(2\alpha/E)^{1/2}a_o^2 \tag{1}$$

where ζ is the excess nuclear charge, α is the dipole polarizability, E is the energy of relative motion, and α and E are measured in atomic units. The corresponding rate coefficient k is

$$k = 3.85 \times 10^{-8} \zeta (\alpha m/\mu)^{1/2} \text{ cm}^3\text{s}^{-1}, \tag{2}$$

where μ/m is the reduced mass expressed in terms of the electron mass, m. For ions of iron interacting with atomic hydrogen

$$k = 1.92 \times 10^{-9} \zeta \text{ cm}^3\text{s}^{-1}, \tag{3}$$

and with atomic helium

$$k = 0.54 \times 10^{-9} \zeta \text{ cm}^3\text{s}^{-1}. \tag{4}$$

Figure 1 compares Equation (3) with the available data for hydrogen charge transfer with the first four ionization stages of the thirty lightest elements compiled by Kingdon & Ferland (1996). The figure indicates the means and the sample standard deviations of these points. Expression (3) is an upper limit that should become more accurate as ζ increases.

3. Applications

We consider the abundance of Fe^{5+} in a collisionally-ionized plasma. The temperatures at which Fe^{5+} is the most abundant ionization stage of iron lie between 1×10^5 K and 2×10^5 K. At 10^5 K, the rate coefficient for radiative and dielectronic recombination of Fe^{5+} is 1×10^{-11} cm^3 s^{-1} (Arnaud & Raymond 1992) and the rate coefficient for charge transfer recombination is about 1×10^{-8} cm^3 s^{-1}. Thus, charge transfer recombination would be comparable only if the neutral hydrogen fraction exceeded 1×10^{-3}. In equilibrium, the neutral hydrogen fraction at this temperature is 1.7×10^{-5} (Arnaud & Rothenflug 1985).

The situation is very different in a cosmic plasma ionized by high frequency photons. The photoionization cross section of atomic hydrogen decreases with frequency ν as $\nu^{-3.5}$ (as $\nu^{-3.3}$ near 1 keV) and the photons are preferentially absorbed by heavy elements producing a plasma in which the hydrogen is partly neutral and Auger ionization creates multiply-ionized heavy elements.

We consider a cell of gas exposed to a blackbody radiation field at a temperature of $\sim 10^6$ K. We adopt the photoionization cross sections listed by Verner & Yakovlev (1995) and Verner et al. (1996) and Auger yields listed by Kaastra & Mewe (1993). We included charge transfer of low ionization stages of Fe, up to Fe^{4+}, with hydrogen (Neufeld & Dalgarno 1989; Kingdon & Ferland 1996). We explored the effects of charge transfer of more highly charged ions by carrying out calculations with rate coefficients given by Equation (3) and with rate coefficients set equal to zero. Figure 2 shows the distribution of ionized stages of Fe for various values of the ionization parameter, U, defined as the ratio of the ionizing photon density to the electron density. Results for six values of U are shown, corresponding to a range from nearly neutral gas to a fully ionized gas. Charge transfer is unimportant for the highest ionization parameter U because with it

the hydrogen is almost completely ionized, but as U diminishes charge transfer causes a major redistribution of the ionization and the abundances of the high ionization stages are greatly reduced. The inclusion of charge transfer with helium modifies the ionization balance by 1% only, due to the smaller rate coefficients and lower abundance compared to hydrogen. We note that a factor of 2 uncertainty in the charge transfer rate coefficient in Equations (3) and (4) will translate into a factor of $\sim 2^n$ uncertainty in the ionic fractions of those ions of excess charge $\zeta = n + 5$, $n \geq 1$.

To illuminate the astrophysical impact of this charge transfer process, we have looked at the infrared lines recently detected in planetary nebula NGC 6302 using the Infrared Space Observatory (Pottasch et al. 1996). The observed intensities of lines [Ne II], [Ne III], [Ne V], [Ne VI], [Mg V], [Mg VI], [Mg VIII], [Ar II], [Ar V] were modeled by Pottasch et al. (1996) using the photoionization code "Cloudy" (Ferland 1993). We applied a model described by Pottasch et al. but included the new charge transfer recombination rates. While the low ionization lines were not affected, some of the high ionization lines changed considerably. The theoretical [Mg V] intensity increased by a factor of 1.7, whereas the [Mg VII] and [Mg VIII] intensities decreased by factors 2.5 and 4.0, respectively. The [Ne VI] and [Na VI] line intensities were reduced by factors of 1.2 and 1.5, respectively, and the [Ar V] line intensity was enhanced by a factor of 2.5. The predicted intensity of the strongest line in the spectrum, [Ne V] 14.32 μm was virtually unaltered. New models that include charge transfer to highly ionized systems are needed to derive the abundances from the observed high ionization lines.

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Fig. 1.— Comparison between the rate coefficients for charge transfer with hydrogen. The line indicates the statistical rate coefficient we adopt for species more than four times charged. The points indicate the mean and standard deviation for charge transfer rate coefficients between hydrogen and the first thirty elements, as given in Kingdon & Ferland (1996).

Fig. 2.— Ionization distributions for iron. Each panel shows results for the ionization parameter indicated, photoionization by a $10^{6.5}$ K blackbody, both with (solid) and without (dotted) the charge transfer rates from Equation (3).